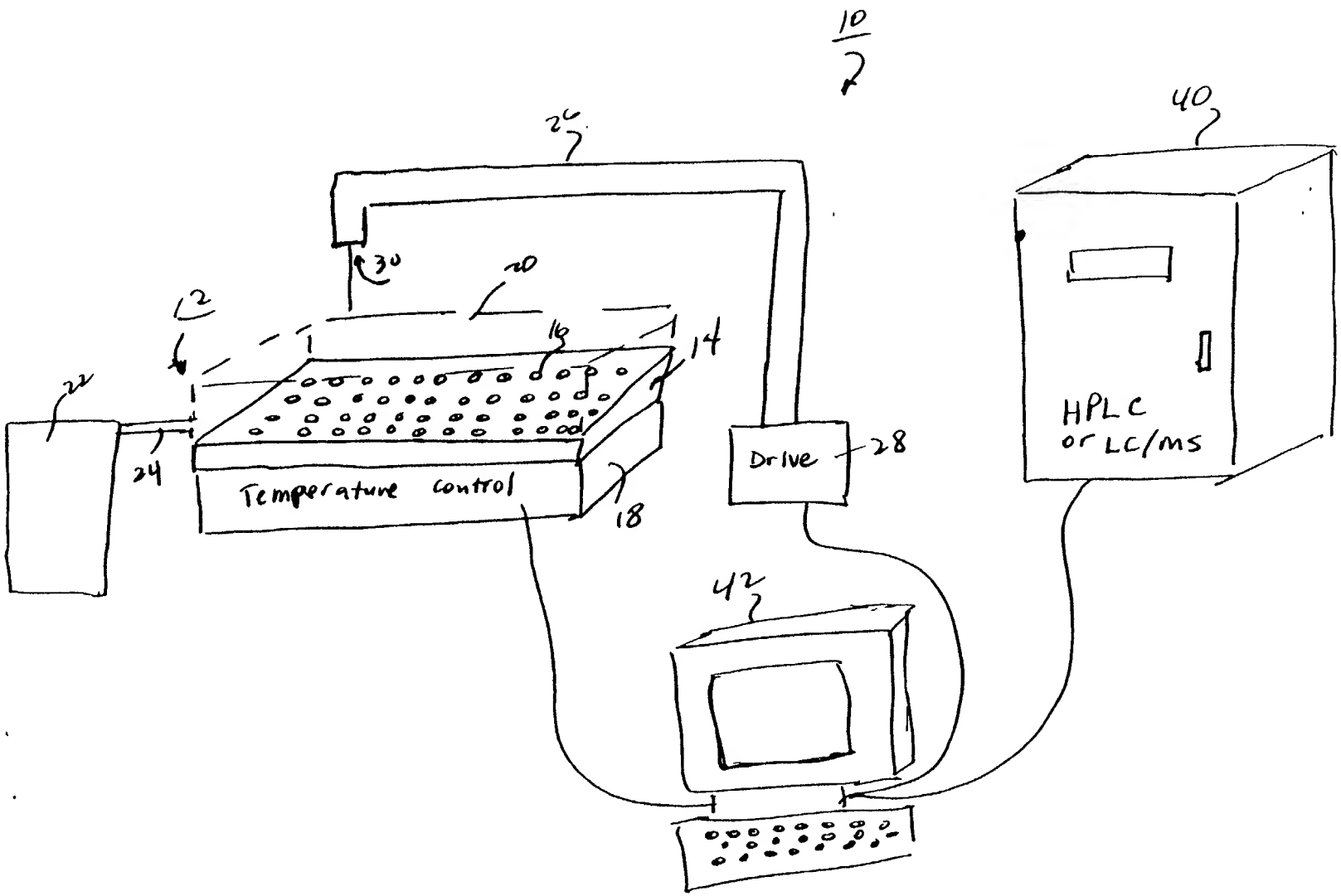

10
26
40
30
20
12
16
14
22
24
Temperature control
18
Drive
28
HPLC
or LC/MS
42

FIG. 1

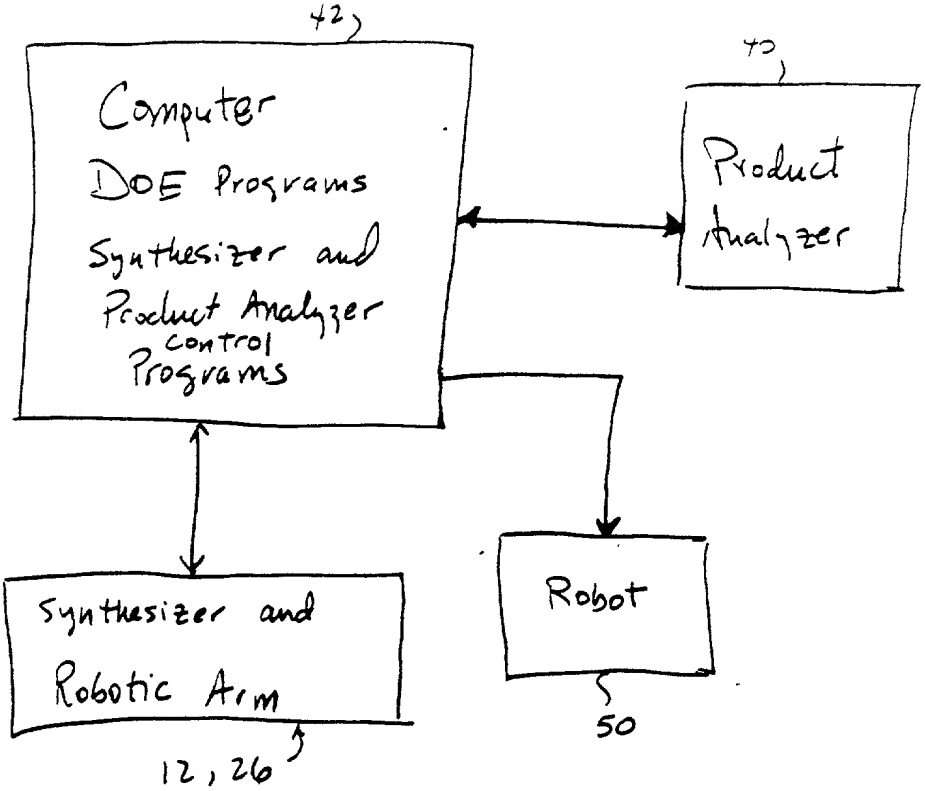

42
Computer
DOE Programs
Synthesizer and
Product Analyzer
control
Programs
40
Product
Analyzer
Synthesizer and
Robotic Arm
12, 26
Robot
50

FIG. 2

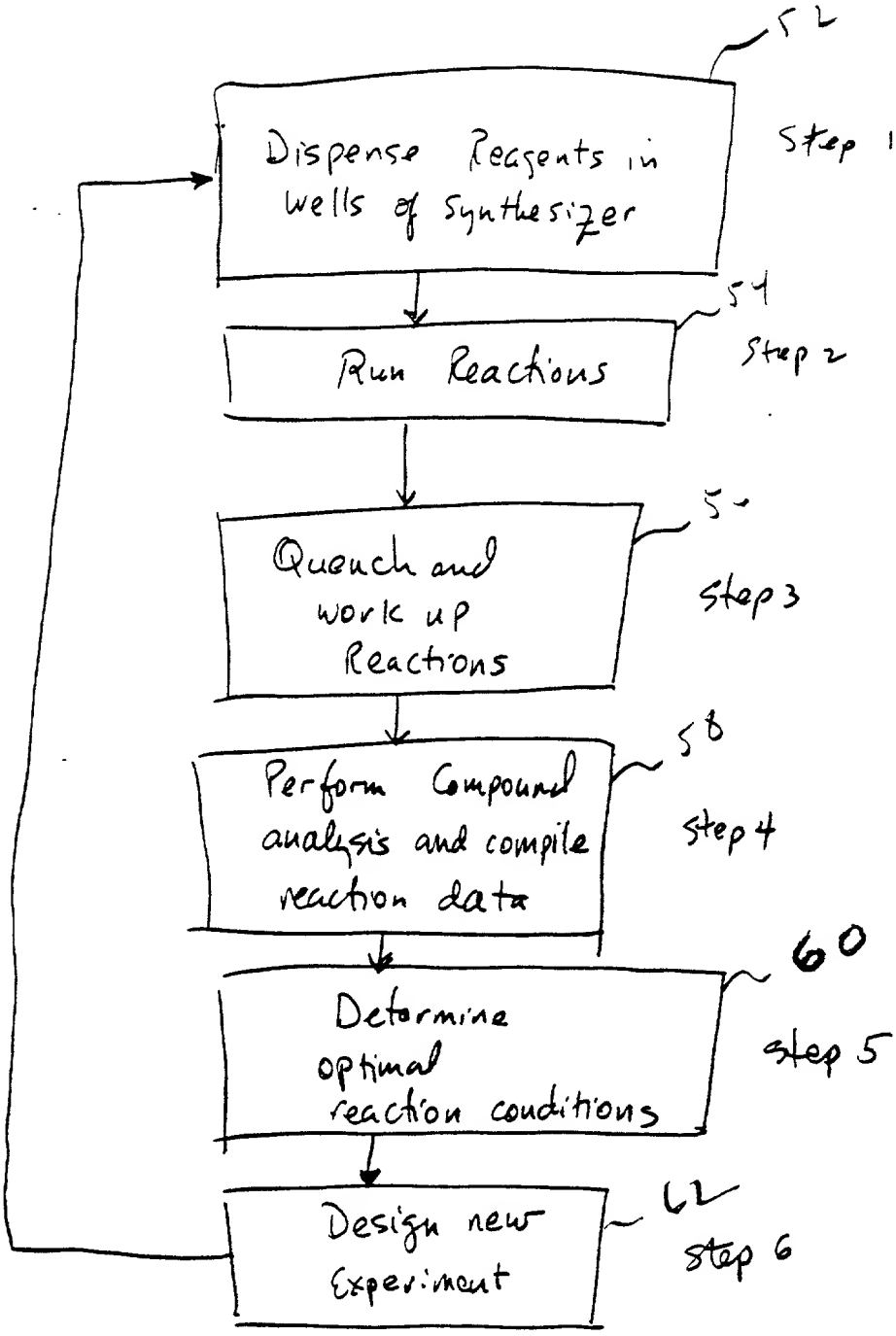

52
Dispense Reagents in wells of Synthesizer
Step 1
54
Run Reactions
Step 2
56
Quench and work up Reactions
Step 3
58
Perform Compound analysis and compile reaction data
Step 4
60
Determine optimal reaction conditions
Step 5
62
Design new Experiment
Step 6

FIG. 3

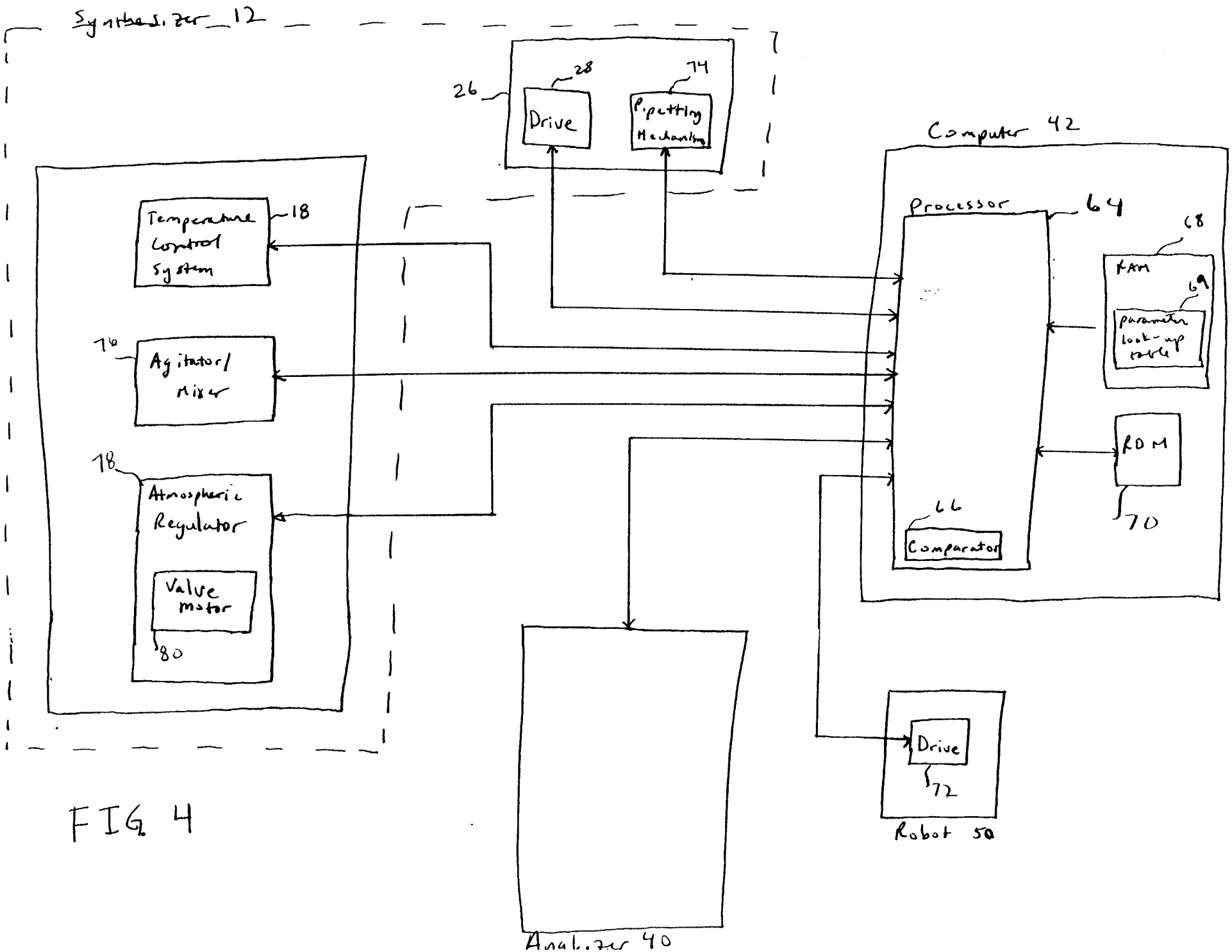
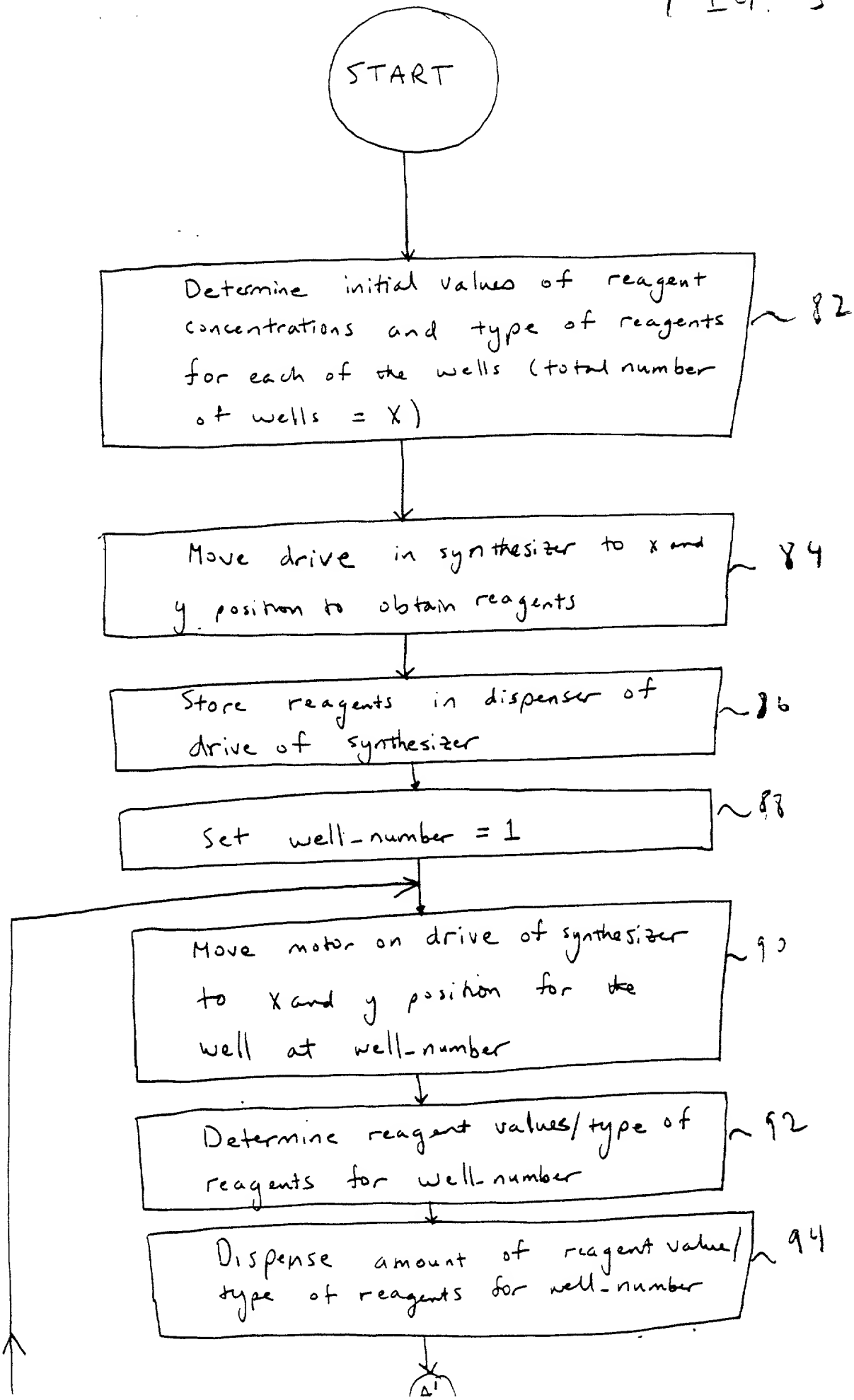
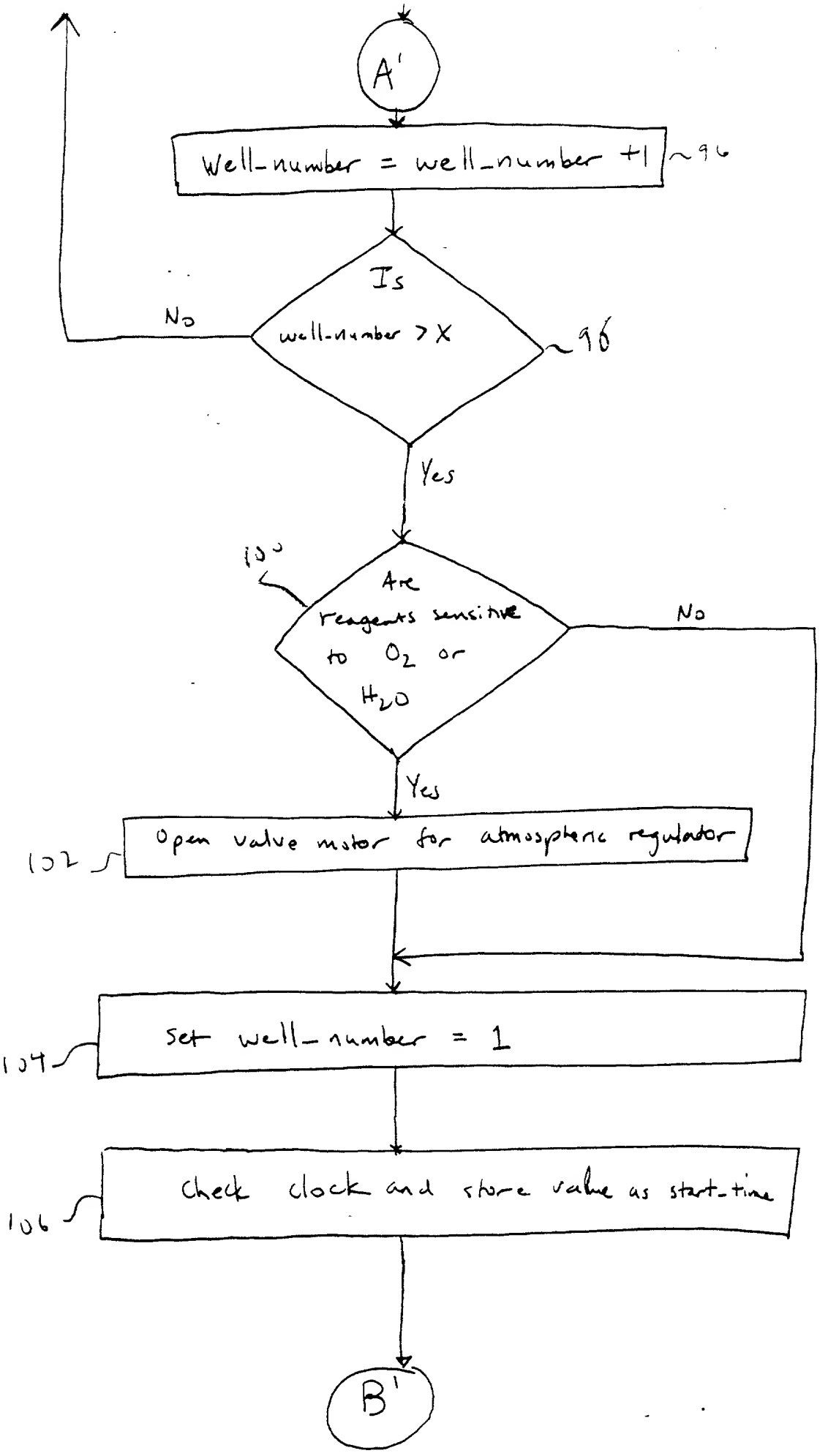
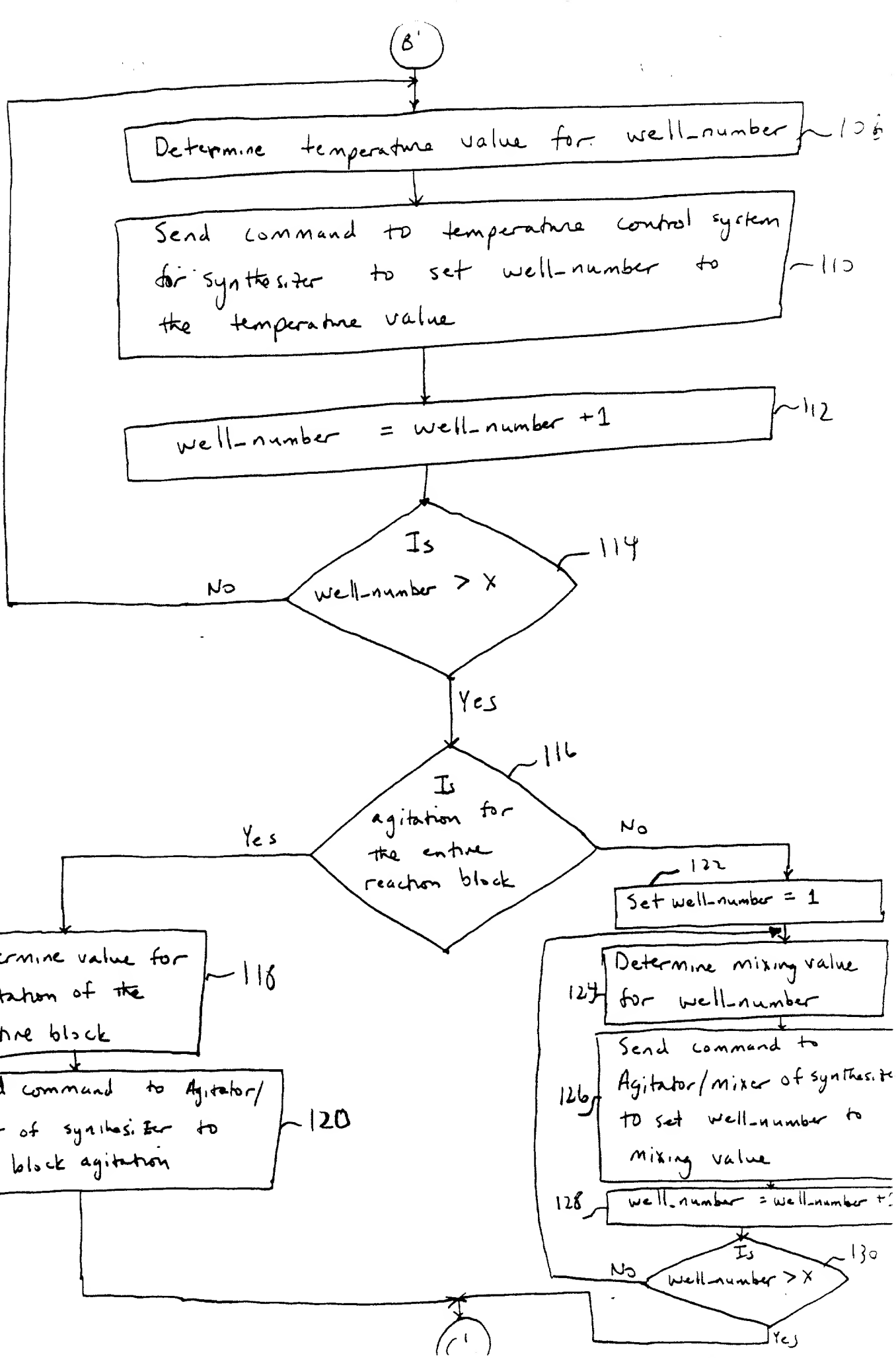

Synthesizer 12
26
28
Drive
74
Pipetting Mechanism
Computer 42
Processor
64
68
RAM
69
parameter look-up table
ROM
70
66
Comparator
Temperature Control System
18
76
Agitator/ Mixer
78
Atmospheric Regulator
Valve motor
80
Drive
72
Robot 50
Analyzer 40

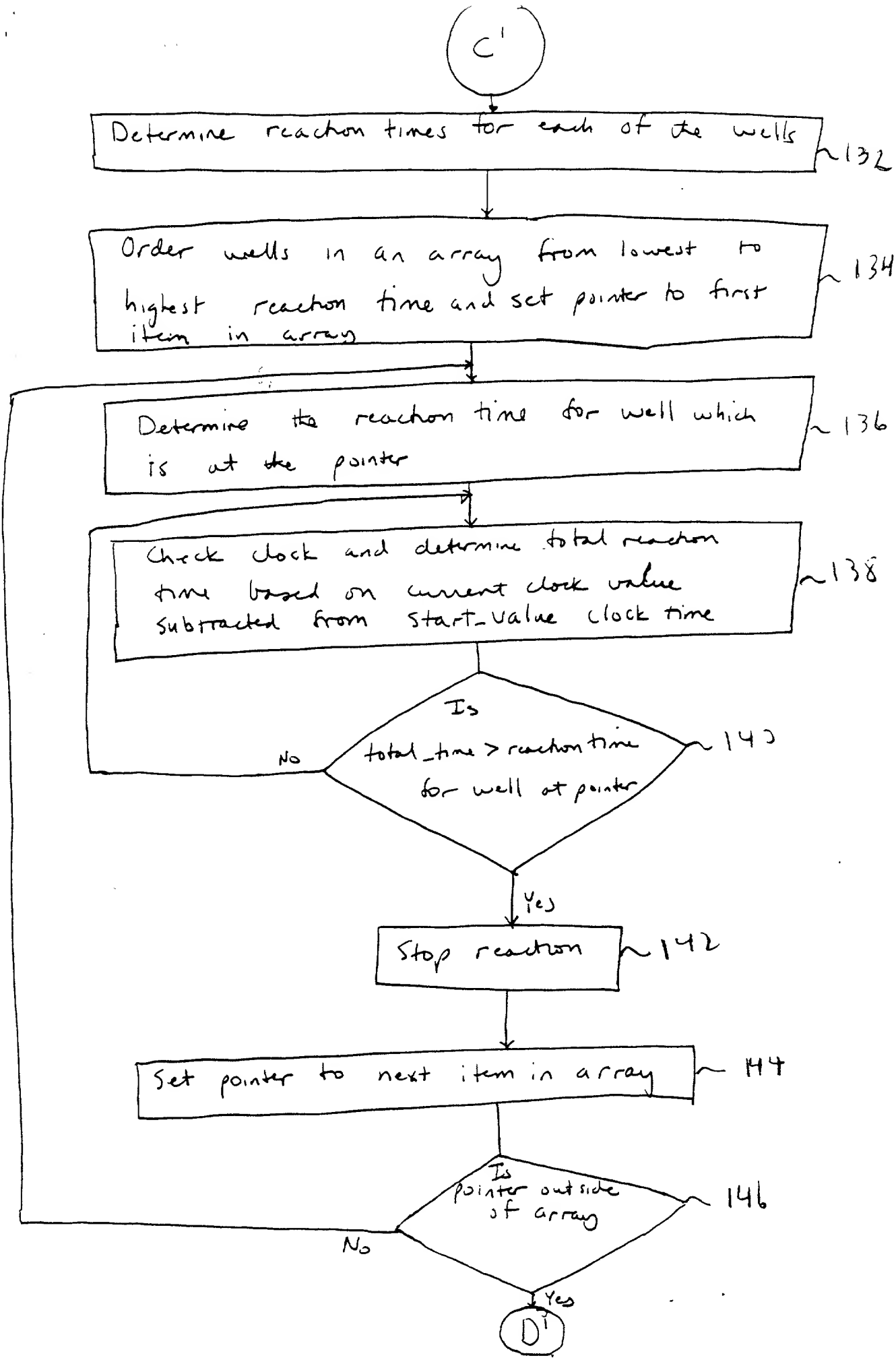
FIG 4

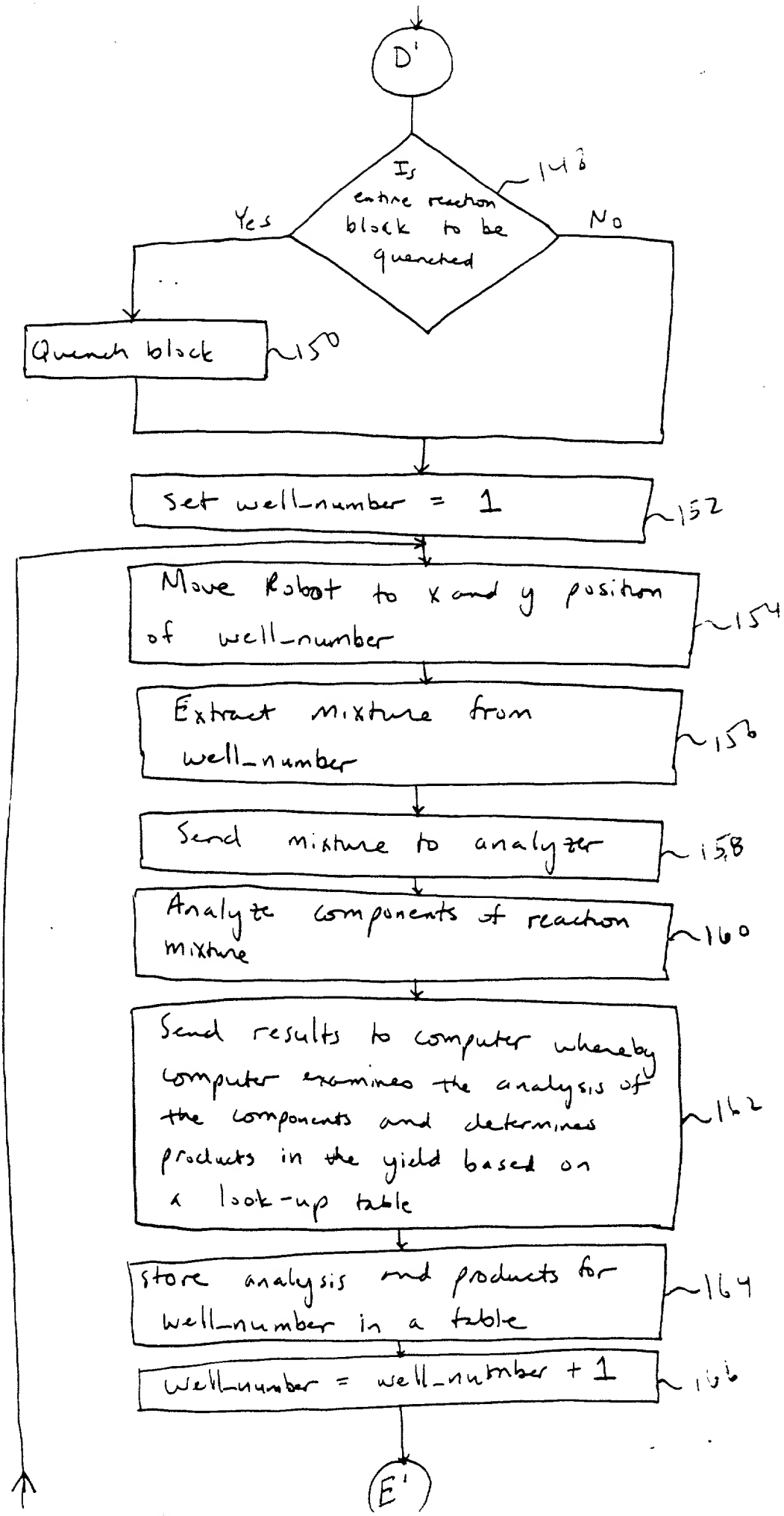
FIG. 5

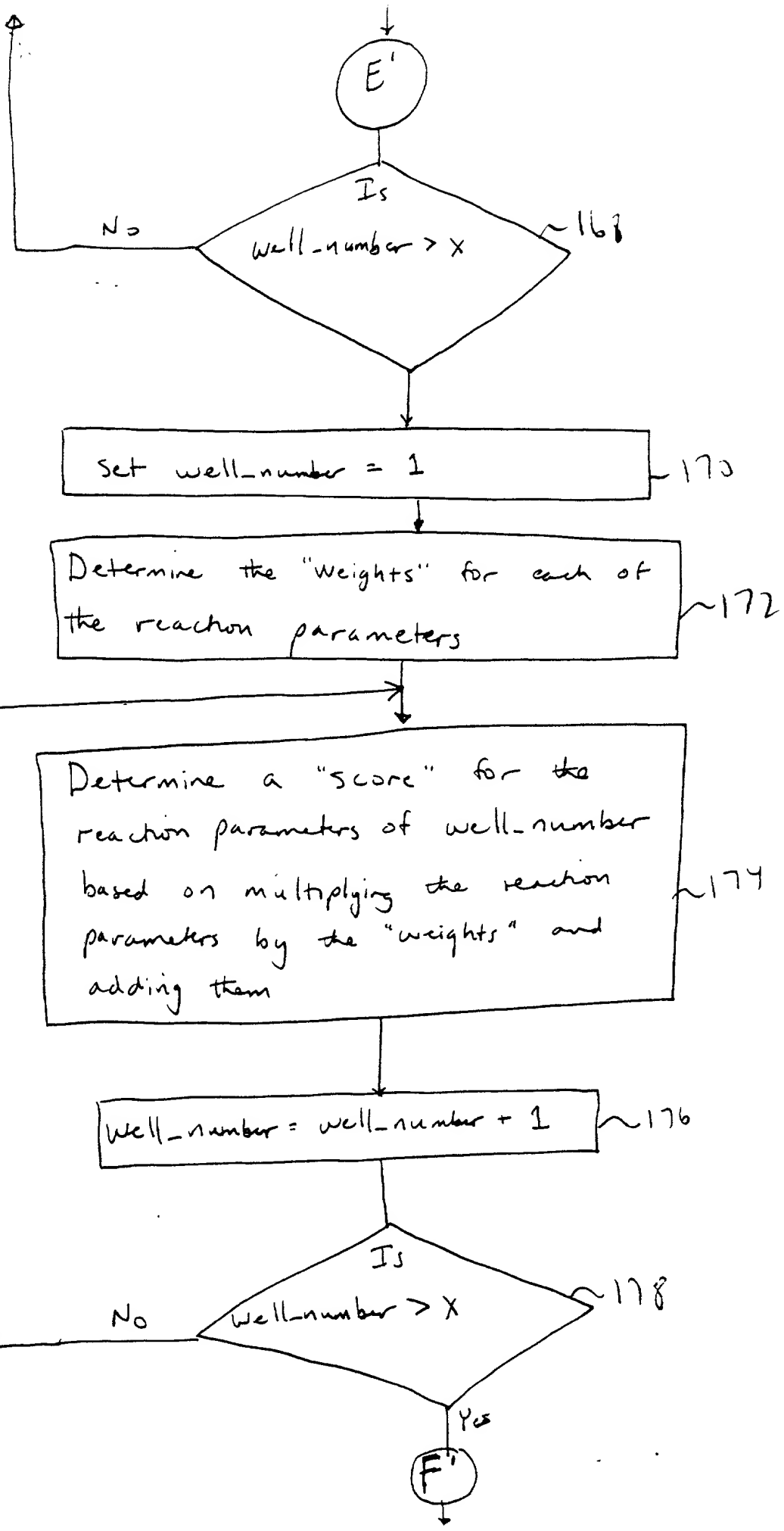

START
Determine initial values of reagent concentrations and type of reagents for each of the wells (total number of wells = X)
82
Move drive in synthesizer to x and y position to obtain reagents
84
Store reagents in dispenser of drive of synthesizer
86
Set well_number = 1
88
Move motor on drive of synthesizer to X and y position for the well at well_number
90
Determine reagent values/type of reagents for well_number
92
Dispense amount of reagent value/type of reagents for well_number
94
A'

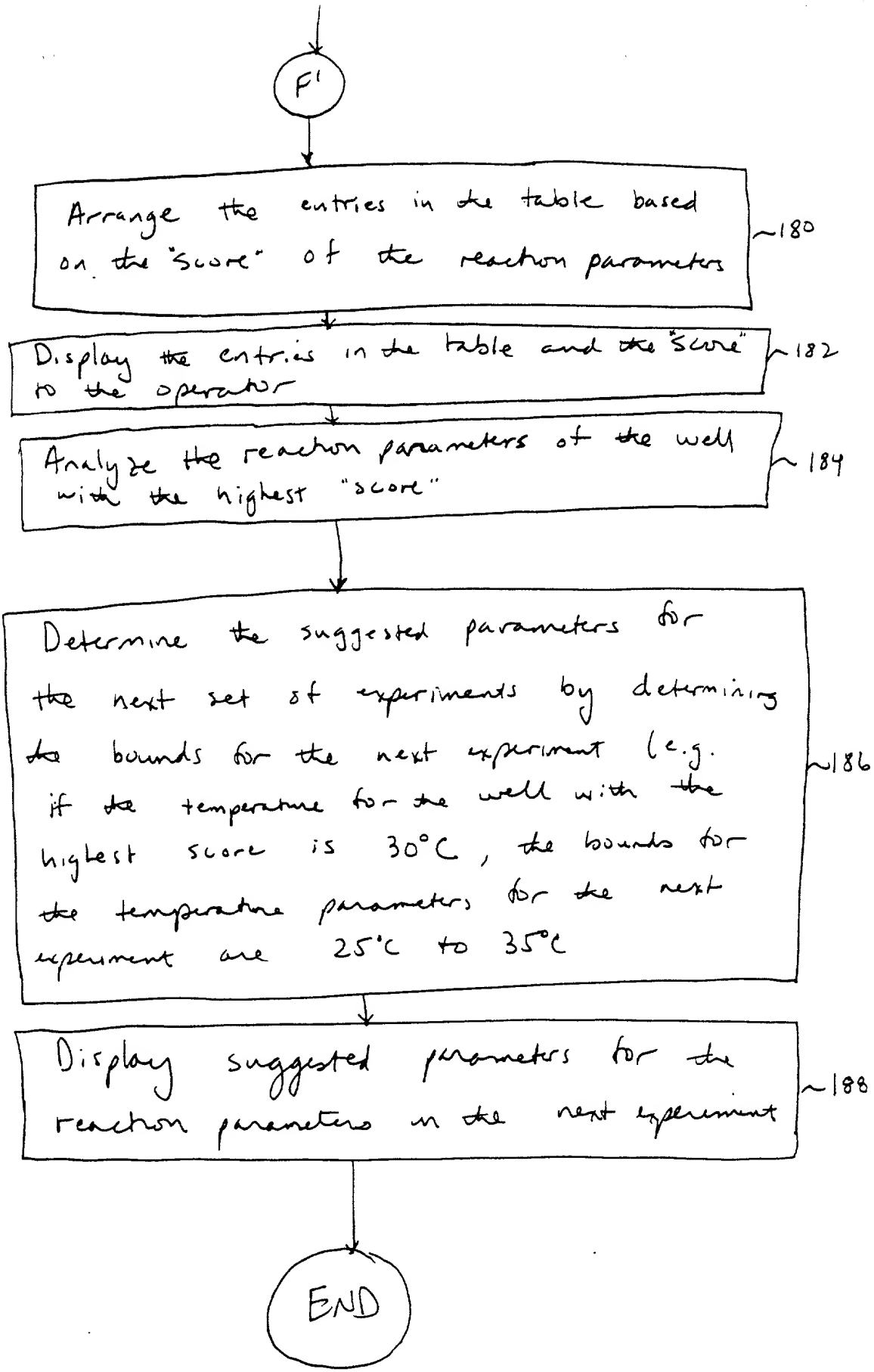

A'
Well_number = well_number +1
96
Is well_number > X
No
96
Yes
100
Are reagents sensitive to O_2 or H_2O
No
Yes
102
Open valve motor for atmospheric regulator
104
Set well_number = 1
106
Check clock and store value as start_time
B'


B'
Determine temperature value for well_number
106
Send command to temperature control system for synthesizer to set well_number to the temperature value
110
well_number = well_number +1
112
Is well_number > X
114
No
Yes
Is agitation for the entire reaction block
116
Yes
No
Determine value for agitation of the entire block
118
Send command to Agitator/ Mixer of synthesizer to set block agitation
120
122
Set well_number = 1
Determine mixing value for well_number
124
Send command to Agitator/mixer of synthesizer to set well_number to mixing value
126
well_number = well_number +1
128
Is well_number > X
130
No
Yes
A'


C'
Determine reaction times for each of the wells
132
Order wells in an array from lowest to highest reaction time and set pointer to first item in array
134
Determine the reaction time for well which is at the pointer
136
Check clock and determine total reaction time based on current clock value subtracted from start_value clock time
138
Is total_time > reaction time for well at pointer
140
No
Yes
Stop reaction
142
Set pointer to next item in array
144
Is pointer outside of array
146
No
Yes
D'


D'
Is entire reaction block to be quenched
148
Yes
No
Quench block
150
Set well_number = 1
152
Move Robot to x and y position of well_number
154
Extract mixture from well_number
156
Send mixture to analyzer
158
Analyze components of reaction mixture
160
Send results to computer whereby computer examines the analysis of the components and determines products in the yield based on a look-up table
162
Store analysis and products for well_number in a table
164
well_number = well_number + 1
166
E'


E'
Is well_number > X
No
168
Set well_number = 1
170
Determine the "weights" for each of the reaction parameters
172
Determine a "score" for the reaction parameters of well_number based on multiplying the reaction parameters by the "weights" and adding them
174
well_number = well_number + 1
176
Is well_number > X
No
178
Yes
F'


F'
Arrange the entries in the table based on the "score" of the reaction parameters
180
Display the entries in the table and the "score" to the operator
182
Analyze the reaction parameters of the well with the highest "score"
184
Determine the suggested parameters for the next set of experiments by determining the bounds for the next experiment (e.g. if the temperature for the well with the highest score is 30°C, the bounds for the temperature parameters for the next experiment are 25°C to 35°C
186
Display suggested parameters for the reaction parameters in the next experiment
188
END